

What is claimed is:

1. A simulation method for partitioning chemical and/or enzyme reaction formulas into two phases: the binding phase where an enzyme  
5 [E] binds to a substrate [S] to form a complex [E:S], and the reaction phase where the complex [E:S] is reacted to produce a product [P], comprising the steps for:

applying numerical formula conversion processing to the binding phase;

- 10 applying numerical formula conversion processing to the reaction phase;

calculating the binding phase using the converted numerical equations;

- 15 calculating the reaction phase using the converted numerical equations.

2. A simulation method as claimed in claim 1, further comprising the steps for:

- 20 generating automatically simultaneous algebraic equations with a binding association constant  $K_b$  in the step for applying numerical formula conversion processing to the binding phase;

- generating automatically a mass balance equation for each basic component that cannot be divided any more in the step for applying numerical formula conversion processing to the binding  
25 phase.

3. A simulation method as claimed in claim 1, further comprising the steps for:

- 30 generating automatically the reaction phase with differential equations in the step for applying numerical formula conversion processing to the reaction phase.

4. A simulation method as claimed in claim 1 for deriving

transcription-translation rate equations from chemical reaction formulas that express that a gene is transcribed into a mRNA and the mRNA is translated into a protein, comprising the steps for:

- extracting chemical reaction equations involving protein synthesis and degradation out of the reaction phase and adding the equations to the transcription-translation rate equations;
- assigning all the transcription-translation equations to the reaction phase.

10 5. A simulator comprising:

- the input part to receive chemical reaction formulas;
- the part for partitioning the enzyme reaction formulas into the biding phase where an enzyme [E] binds to a substrate [S] to form a complex [E:S], and the reaction phase where the complex [E:S]
- 15 is reacted to produce a product [P];
- the part of applying numerical formula conversion processing to the binding phase in order to generate simultaneous algebraic equations;
- the part of applying numerical formula conversion processing
- 20 to the reaction phase in order to generate differential equations;
- the execution part for numerically simulating the binding and reaction phases based on the converted equations;
- the output part of the result of simulation.

25 6. Computer-readable media recording the programs that enforce the present invention, comprising the steps for:

- partitioning the chemical and/or enzyme reaction formulas into the biding phase where an enzyme [E] binds to a substrate [S] to form a complex [E:S], and the reaction phase where the complex
- 30 [E:S] is reacted to produce a product [P];
- applying numerical formula conversion processing to the binding phase in order to generate simultaneous algebraic equations;

